

FIG. 1

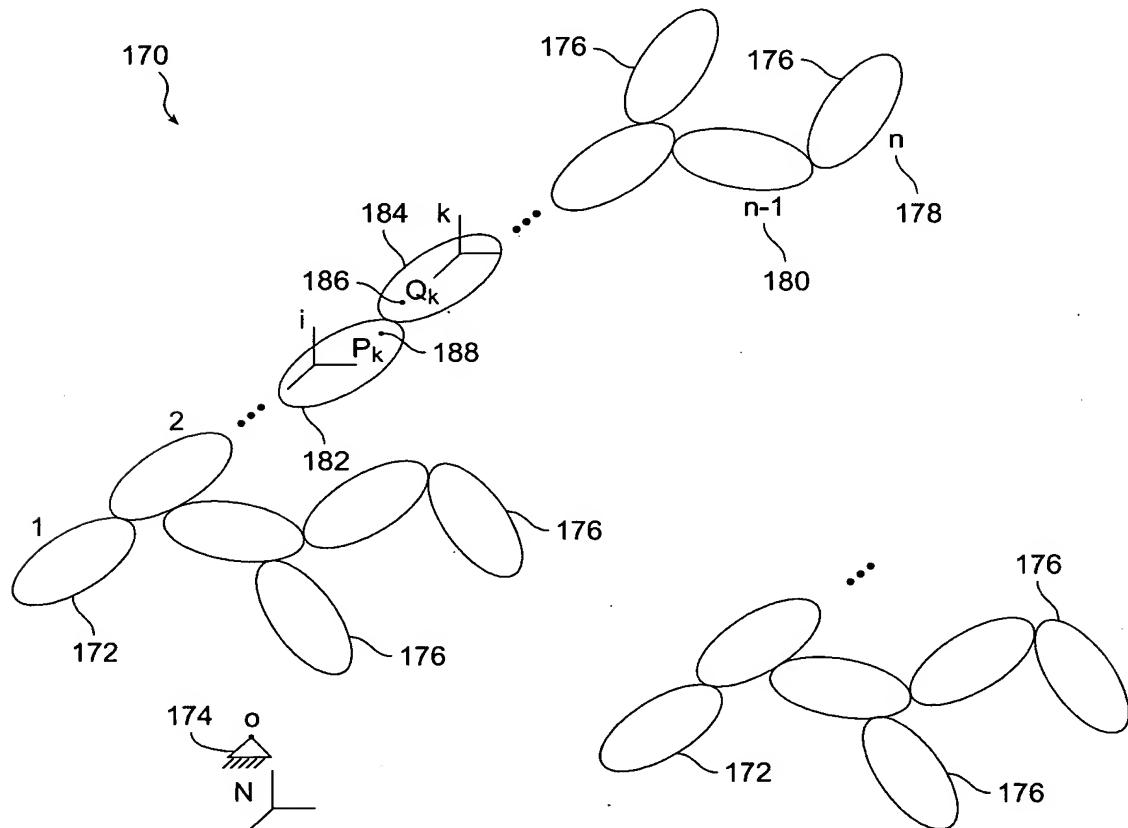


FIG. 2

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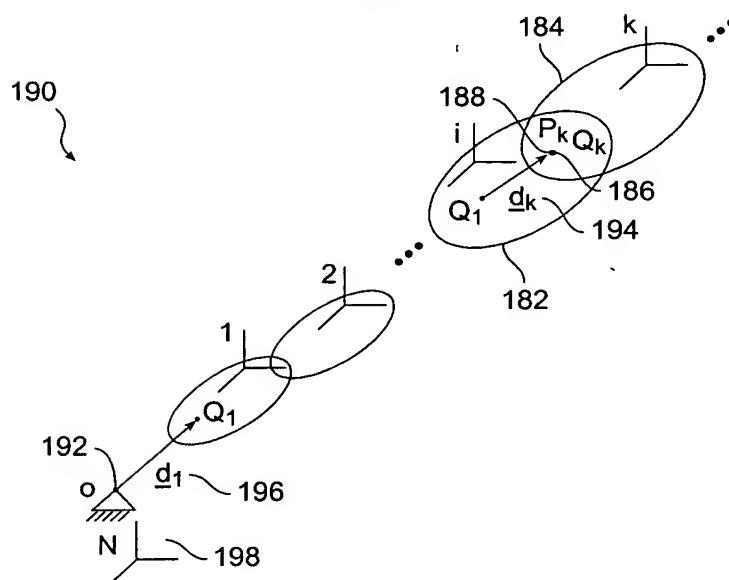


FIG. 3

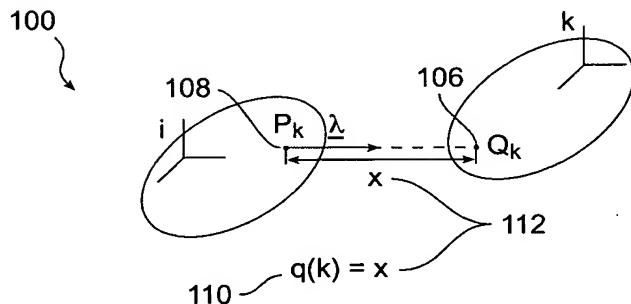


FIG. 4A

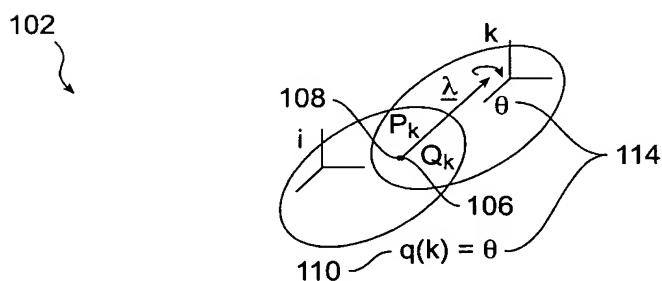


FIG. 4B

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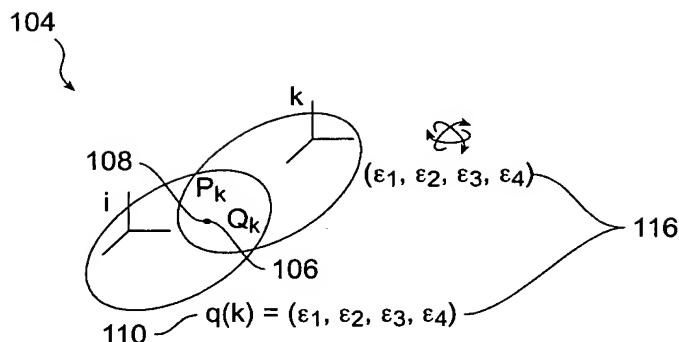


FIG. 4C

RESIDUAL FORM METHOD TO COMPUTE $\rho_q$ AND $\rho_u$	DIRECT FORM METHOD TO COMPUTE $\dot{q}$ AND $\dot{u}$
<ol style="list-style-type: none"> <li>1. COMPUTE THE FIRST KINEMATICS CALC. AND THE FIRST KINEMATIC RESIDUAL <math>\rho_q(k)</math></li> <li>2. GENERATE <math>\hat{T}(k)</math>, THE SPACIAL LOAD BALANCE FOR EACH BODY</li> <li>3. COMPUTE DYNAMIC RESIDUAL <math>\rho_u(k)</math></li> </ol>	<ol style="list-style-type: none"> <li>1. COMPUTE <math>\dot{q}</math> USING JOINT SPECIFIC ROUTINES</li> <li>2. PERFORM FIRST KINEMATICS CALC. WITH <math>\dot{u} = 0</math></li> <li>3. GENERATE RESIDUALS <math>\rho_u</math> AND NEGATE <math>\rho_u = -\rho_u</math></li> <li>4. PERFORM SECOND KINEMATICS CALC.</li> <li>5. COMPUTE <math>\dot{u}</math> USING FORWARD DYNAMICS</li> </ol>

COMPARISON OF METHODS

FIG. 5

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MOLECULE	NO. RESIDUES IN POLYPEPTIDE	NO. ATOMS	DIRECT FORM APPROXIMATE OPERATION COUNT	RESIDUAL FORM APPROXIMATE OPERATION COUNT	FACTOR OF SPEED UP
ALANINE DIPEPTIDE	2	23	4,991	683	7.31
20-MER POLYALANINE	20	257	42,340	5,894	7.24
100-MER POLYALANINE	100	1297	207,018	28,973	7.15

COMPUTATION COMPARISON

FIG. 6